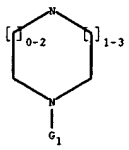
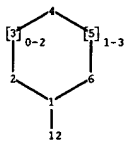
C:\STNEXP4\QUERIES\099345[redacted].str





search of applicants species

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ring nodes :
    1  2  3  4  5  6
ring/chain nodes :
    12
chain bonds :
    1-12
ring bonds :
    1-2  1-6  2-3  3-4  4-5  5-6
exact/norm bonds :
    1-2  1-6  1-12  2-3  3-4  4-5  5-6
isolated ring systems :
    containing 1 :


G1:Cy,O,S,N,Se

Match level :
    1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  12:CLASS
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=> d his

     (FILE 'HOME' ENTERED AT 11:38:28 ON 28 APR 2003)

     FILE 'REGISTRY' ENTERED AT 11:38:34 ON 28 APR 2003
L1              STRUCTURE UPLOADED
L2              QUE L1
L3         134192 S 7/SZ
L4             50 S L2  SUB=L3 SAM
L5              1 S DIAZEPINE/CN
L6          23917 S C5N2/EA
L7          23917 S L3 AND L6
L8             50 S L2  SUB=L7 SAM

     FILE 'HCAPLUS' ENTERED AT 11:43:11 ON 28 APR 2003
L9              1 S 133:321908/DN
                SELECT RN L9 1-

     FILE 'REGISTRY' ENTERED AT 11:43:56 ON 28 APR 2003
L10           256 S E1-256
L11           206 S L3 AND L10

     FILE 'CAPLUS' ENTERED AT 11:46:04 ON 28 APR 2003
L12           486 S L11
L13           ANALYZE L12 1- RN HIT :     206 TERMS

     FILE 'REGISTRY' ENTERED AT 11:46:54 ON 28 APR 2003
L14             1 S 505-66-8/RN
L15             1 S 112275-50-0/RN
L16               STRUCTURE UPLOADED
L17               QUE L16
L18            50 S L17  SUB=L7 SAM
L19           204 S L11 NOT (L14 OR L15)
L20          8857 S L17  SUB=L7 FUL

     FILE 'CAPLUS' ENTERED AT 11:50:58 ON 28 APR 2003
L21          1428 S L20
L22             7 S L19
L23           ANALYZE L21 1- RN HIT :    5673 TERMS

     FILE 'REGISTRY' ENTERED AT 11:52:58 ON 28 APR 2003
L24             1 S 80755-51-7/RN
L25             1 S 103745-39-7/RN
L26             1 S 87233-62-3/RN
L27             1 S 87233-61-2/RN
L28             1 S 105637-50-1/RN
L29             1 S 52712-76-2/RN
L30             1 S 109376-83-2/RN
L31             1 S 105628-72-6/RN
L32             1 S 211872-02-5/RN
L33             1 S 105628-07-7/RN
L34          8847 S L21 NOT (L24 OR L25 OR L26 OR L27 OR L28 OR L29 OR L30 OR L31

     FILE 'CAPLUS' ENTERED AT 11:58:29 ON 28 APR 2003
L35           987 S L34

     FILE 'REGISTRY' ENTERED AT 11:59:33 ON 28 APR 2003
L36             STRUCTURE UPLOADED
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L37             QUE L36
L38          840 S L37  SUB=L20 FUL
L39         8017 S L20 NOT L38

     FILE 'CAPLUS' ENTERED AT 12:00:48 ON 28 APR 2003

     FILE 'REGISTRY' ENTERED AT 12:03:58 ON 28 APR 2003
L40             STRUCTURE UPLOADED
L41             QUE L40
L42         3353 S L41  SUB=L20 FUL
L43         5504 S L20 NOT L42
L44         4780 S L43 NOT L38

     FILE 'CAPLUS' ENTERED AT 12:05:14 ON 28 APR 2003
L45          884 S L44
L46          ANALYZE L45 1- RN HIT :    4349 TERMS

     FILE 'REGISTRY' ENTERED AT 12:06:31 ON 28 APR 2003

     FILE 'CAPLUS' ENTERED AT 12:06:32 ON 28 APR 2003

     FILE 'REGISTRY' ENTERED AT 12:11:06 ON 28 APR 2003
L47             1 S 101954-20-5/RN
L48             1 S 41578-59-0/RN
L49             1 S 55557-00-1/RN
L50             1 S 5754-90-5/RN
L51             1 S 122423-30-7/RN
L52             1 S 122423-29-4/RN
L53             1 S 21091-66-7/RN
L54               STRUCTURE UPLOADED
L55               QUE L54
L56         4223 S L55  SUB=L44 FUL

     FILE 'CAPLUS' ENTERED AT 12:15:43 ON 28 APR 2003
L57          729 S L56

     FILE 'REGISTRY' ENTERED AT 12:16:35 ON 28 APR 2003

     FILE 'CAPLUS' ENTERED AT 12:16:36 ON 28 APR 2003

     FILE 'REGISTRY' ENTERED AT 12:16:42 ON 28 APR 2003

     FILE 'CAPLUS' ENTERED AT 12:16:43 ON 28 APR 2003

     FILE 'REGISTRY' ENTERED AT 12:16:46 ON 28 APR 2003
L58         4217 S L56 NOT (L47 OR L48 OR L49 OR L50 OR L51 OR L52 OR L53)

     FILE 'CAPLUS' ENTERED AT 12:17:59 ON 28 APR 2003
L59          706 S L58

     FILE 'REGISTRY' ENTERED AT 12:18:46 ON 28 APR 2003
L60          188 S L11 AND L58
L61           18 S L11 NOT L60

     FILE 'CAPLUS' ENTERED AT 12:20:29 ON 28 APR 2003

=> d bib abs hitstr l22 1-7
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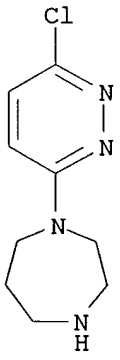
L22 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2003 ACS
AN 2002:558408 CAPLUS
DN 137:257238
TI 6-Chloropyridazin-3-yl Derivatives Active as Nicotinic Agents: Synthesis, Binding, and Modeling Studies
AU Toma, Lucio; Quadrelli, Paolo; Bunnelle, William H.; Anderson, David J.; Meyer, Michael D.; Cignarella, Giorgio; Gelain, Arianna; Barlocco, Daniela
CS Dipartimento di Chimica Organica, Universita di Pavia, Pavia, 27100, Italy
SO Journal of Medicinal Chemistry (2002), 45(18), 4011-4017
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB 3,8-Diazabicyclo[3.2.1]octane (1), 2,5-diazabicyclo[2.2.1]heptane (2), piperazine (3), and homopiperazine (4) derivs., substituted at one nitrogen atom with the 6-chloro-3-pyridazinyl group while the other nitrogen atom was either unsubstituted or mono- or dimethylated, were synthesized and tested for their affinity toward the neuronal nicotinic acetylcholine receptors (nAChRs). All of the compds. had Ki values in the nanomolar range. A mol. modeling study allowed location of their preferred conformations, the energies of which were recalcd. in water with a continuum solvent model. Some of the compds. showed, in their populated conformations, only pharmacophoric distances longer than the values taken into consideration by the Sheridan model for nAChRs receptors. Thus, this SAR study gives support to the hypothesis that these longer distances are still compatible with affinity for .alpha.4.beta.2 receptors in the nanomolar range.
IT **100224-61-1P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(6-chloropyridazin-3-yl derivs. active as nicotinic agents: prepn., binding, and modeling study)
RN 100224-61-1 CAPLUS
CN 1H-1,4-Diazepine, 1-(6-chloro-3-pyridazinyl)hexahydro- (9CI) (CA INDEX NAME)

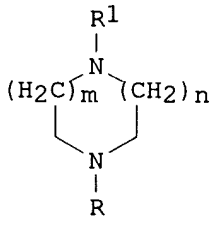


RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2003 ACS
AN 2002:293427 CAPLUS
DN 136:325574
TI Preparation of piperazine, homopiperazine, and 8-azabicyclo[3.2.1]oct-2-ene, and 3,9-diazabicyclo[4.2.1]nonane derivatives for treatment of affective disorders by the combined action of a nicotinic receptor agonist and a monoaminergic substance
IN Olsen, Gunnar M.; Peters, Dan; Nielsen, Elsebet Ostergaard
PA Neurosearch A/S, Den.
SO PCT Int. Appl., 31 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002030405	A2	20020418	WO 2001-DK661	20011010
	WO 2002030405	A3	20020906		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2001095436	A5	20020422	AU 2001-95436	20011010
PRAI	DK 2000-1535	A	20001013		
	US 2000-242146P	P	20001023		
	WO 2001-DK661	W	20011010		

OS MARPAT 136:325574
GI



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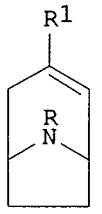


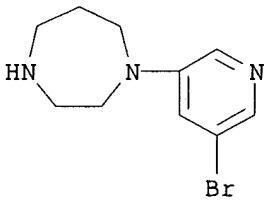
II

AB This invention relates to use of the combined action of a nicotinic acetylcholine receptor agonist and a monoamine reuptake inhibitor for the treatment of affective disorders including depression, anxiety, obsessive compulsive disorder (OCD), panic disorder, or pain, as well as to pharmaceutical compns. comprising these substances and chem. substances for use according to the invention. The chem. substances are represented by piperazine and homopiperazine derivs. (I; n = 1,2,3; m = 0,1,2; R = H, alkyl, cycloalkyl, cycloalkylalkyl, alkoxy, acyl, benzyl; R1 = 5-bromo-3-pyridyl, 6-chloro-3-pyridyl, 6-bromo-5-methoxy-3-pyridyl, 6-bromo-3-pyridyl, 6-bromo-5-chloro-3-pyridyl, 5,6-dibromo-3-pyridyl,

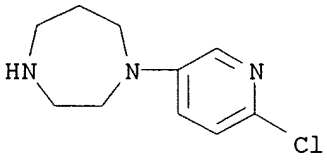
etc.) and 8-azabicyclo[3.2.1]oct-2-ene derivs. (II; R = H, alkyl, alkenyl, cycloalkyl, cyanoalkyl, Ph, naphthyl, benzyl; R1 = CHO, alkanoyl, cycloalkanoyl, carbamoyl, furanyl, thienyl, pyrrolyl, oxazolyl, isoxazolyl, imidazolyl, pyridyl, pyrimidinyl, thiazolyl, naphthyl, indolyl, benzofuranyl, etc.). Thus, 1-(6-Chloro-3-pyridyl)piperazine (III) (0.3, 1, 3, 10 mg/kg s.c.) was tested in the mouse forced swim test which is considered predictive of a potential antidepressant pharmacol. effect and it did not affect forced swimming with a 30 min pretreatment. However, the combination of venlafaxine and III (1+3; 3+3; 10+1; 10+3 mg/kg s.c.) significantly increased the forced swimming in NMRI mice.

IT **223796-92-7P**, 1-(5-Bromo-3-pyridyl)homopiperazine
223797-23-7P, 1-(6-Chloro-3-pyridyl)homopiperazine
303159-57-1P, 1-(5,6-Dichloro-3-pyridyl)homopiperazine
303160-60-3P, 1-(5-Methoxy-6-bromo-3-pyridyl)homopiperazine
303160-62-5P, 1-(5-Methoxy-6-iodo-3-pyridyl)homopiperazine
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of piperazine, homopiperazine, azabicyclo[3.2.1]octene, and diazabicyclo[4.2.1]nonane derivs. for treatment of affective disorders)

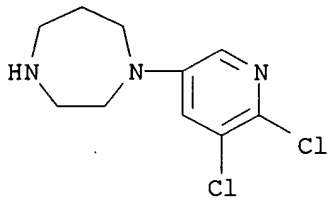
RN 223796-92-7 CAPLUS
CN 1H-1,4-Diazepine, 1-(5-bromo-3-pyridinyl)hexahydro- (9CI) (CA INDEX NAME)



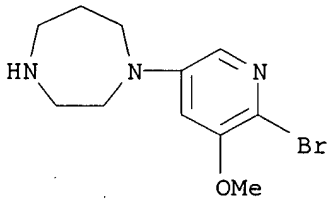
RN 223797-23-7 CAPLUS
CN 1H-1,4-Diazepine, 1-(6-chloro-3-pyridinyl)hexahydro- (9CI) (CA INDEX NAME)



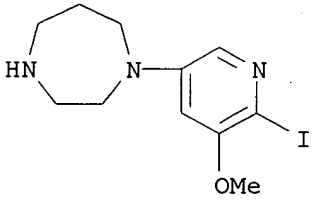
RN 303159-57-1 CAPLUS
CN 1H-1,4-Diazepine, 1-(5,6-dichloro-3-pyridinyl)hexahydro- (9CI) (CA INDEX NAME)



RN 303160-60-3 CAPLUS
CN 1H-1,4-Diazepine, 1-(6-bromo-5-methoxy-3-pyridinyl)hexahydro- (9CI) (CA INDEX NAME)



RN 303160-62-5 CAPLUS
CN 1H-1,4-Diazepine, hexahydro-1-(6-iodo-5-methoxy-3-pyridinyl)- (9CI) (CA INDEX NAME)

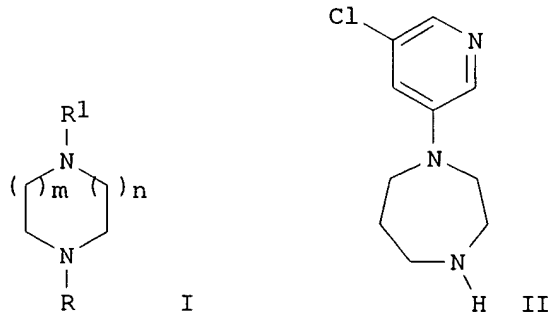


appl.

L22 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2003 ACS
AN 2000:772619 CAPLUS
DN 133:321908
TI Heteroaryl diazacycloalkanes, their preparation, and their use as nicotinic acetylcholine receptor ligands
IN Nielsen, Simon Feldbaek; Peters, Dan; Nielsen, Elsebet Ostergaard; Olsen, Gunnar M.
PA Neurosearch A/S, Den.
SO PCT Int. Appl., 70 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000064885	A1	20001102	WO 2000-DK202	20000419
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	NZ 514021	A	20010928	NZ 2000-514021	20000419
	EP 1175416	A1	20020130	EP 2000-920421	20000419
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	JP 2002543070	T2	20021217	JP 2000-614237	20000419
	US 2002045618	A1	20020418	US 2001-934531	20010823
PRAI	DK 1999-571	A	19990426		
	DK 1999-1504	A	19991020		
	WO 2000-DK202	W	20000419		

OS MARPAT 133:321908
GI

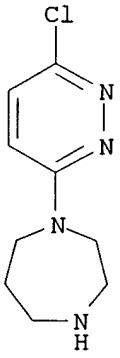


AB The invention relates to novel heteroaryl diazacycloalkane derivs. I and their enantiomers, N-oxides, salts, and/or labeled forms [wherein: n = 1, 2, 3; m = 0, 1, 2; R = H, alkyl, cycloalkyl, cycloalkylalkyl, alkenyl, alkynyl, aralkyl, alkoxypyridyl, alkenyloxypyridyl, or bridging moiety to

form a dimer; R1 = (un)substituted monocyclic 5- or 6-membered heterocyclyl or bicyclic heterocyclyl; or R = R1 = (un)substituted monocyclic 5- or 6-membered heterocyclyl]. The compds. are cholinergic ligands at nicotinic acetylcholine receptors, and may be useful for the treatment of a diversity of diseases and disorders, e.g., those related to the CNS cholinergic system, smooth muscle contraction, the endocrine system, neurodegeneration, inflammation, pain, and substance abuse withdrawal symptoms. A large no. of compds., mostly homopiperazine derivs., were prepd. and/or claimed. For instance, neat reaction of 3,5-dichloropyridine with homopiperazine at 150.degree. gave title compd. II in 40% yield. Similar compds. inhibited binding of 3H-epibatidine to rat brain nicotinic receptors with IC50 values as low as 0.001 .mu.M.

IT **100224-61-1P**, 1-(6-Chloro-3-pyridazinyl)homopiperazine **223796-20-1P**, 1-(3-Pyridyl)homopiperazine **223796-92-7P**, 1-(5-Bromo-3-pyridyl)homopiperazine **223797-48-6P**, 1-(3-Pyridyl)-4-(tert-butoxycarbonyl)homopiperazine **303159-88-8P**, 1-[5-(Phenylacetylenyl)-3-pyridyl]homopiperazine **303159-92-4P**, 1-[5-(1-Methylprop-2-enyloxy)-3-pyridyl]homopiperazine **303160-09-0P**, 1-(6-Amino-3-pyridyl)homopiperazine **303160-10-3P**, 1-(6-Nitro-3-pyridyl)homopiperazine **303160-83-0P**, 1-[5-[5-(1-Homopiperazinyl)pyrid-3-yl]pyrid-3-yl]homopiperazine **303161-25-3P**, 1-(5-Bromo-3-pyridyl)-4-(tert-butoxycarbonyl)homopiperazine **303161-42-4P**, 1-[5-(Prop-1-enyloxy)-3-pyridyl]-4-(tert-butoxycarbonyl)homopiperazine **303161-60-6P**, 1-(5-Iodo-3-pyridyl)-4-(tert-butoxycarbonyl)homopiperazine **303161-61-7P**, 1-[5-(Trimethylstannyl)-3-pyridyl]-4-(tert-butoxycarbonyl)homopiperazine
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; prepn. of heteroaryldiazacycloalkanes as nicotinic acetylcholine receptor ligands)

RN 100224-61-1 CAPLUS
CN 1H-1,4-Diazepine, 1-(6-chloro-3-pyridazinyl)hexahydro- (9CI) (CA INDEX NAME)

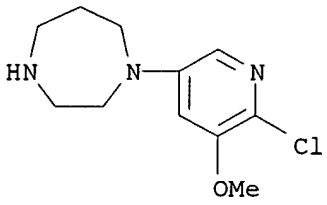


RN 223796-20-1 CAPLUS
CN 1H-1,4-Diazepine, hexahydro-1-(3-pyridinyl)- (9CI) (CA INDEX NAME)

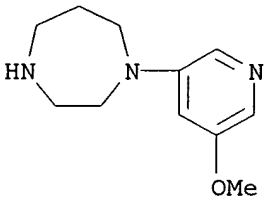
L22 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2003 ACS
AN 2000:553442 CAPLUS
DN 133:168383
TI Pharmaceutical compositions containing nicotine or a ligand of nicotine receptors and a monamine oxidase inhibitor and their use for treating tobacco withdrawal symptoms
IN Caille, Dominique; George, Pascal; Jegham, Samir; Robineau, Pascale; Scatton, Bernard; Zivkovic, Branimir
PA Sanofi-Synthelabo, Fr.
SO PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DT Patent
LA French
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000045846	A1	20000810	WO 2000-FR193	20000128
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	FR 2788982	A1	20000804	FR 1999-1144	19990202
	FR 2788982	B1	20020802		
	EP 1150715	A1	20011107	EP 2000-901660	20000128
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	JP 2002536342	T2	20021029	JP 2000-596965	20000128
PRAI	FR 1999-1144	A	19990202		
	WO 2000-FR193	W	20000128		

OS MARPAT 133:168383
AB The invention concerns novel pharmaceutical compns. contg. nicotine or a ligand of nicotine receptors and a monamine oxidase inhibitor designed for treating tobacco withdrawal symptoms. A bilayer tablet contained befloxatone 5, lactose 66, microcryst. cellulose 20, povidone 4, crospovidone 4, and magnesium stearate 1% in the first layer, and nicotine polacrylix 5, microcryst. cellulose 20 povidone 4, hydroxypropyl Me cellulose 25, magnesium stearate 1, and lactose q.s. 100% in the second layer.
IT **223796-26-7 223796-36-9**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmaceutical compns. contg. nicotine or ligand of nicotine receptors and monamine oxidase inhibitor and their use for treating tobacco withdrawal symptoms)
RN 223796-26-7 CAPLUS
CN 1H-1,4-Diazepine, 1-(6-chloro-5-methoxy-3-pyridinyl)hexahydro- (9CI) (CA INDEX NAME)

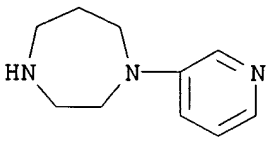


RN 223796-36-9 CAPLUS
CN 1H-1,4-Diazepine, hexahydro-1-(5-methoxy-3-pyridinyl)- (9CI) (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

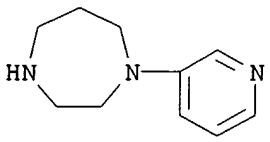
L22 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2003 ACS
AN 2000:293414 CAPLUS
DN 133:99064
TI Novel potent ligands for the central nicotinic acetylcholine receptor: synthesis, receptor binding, and 3D-QSAR analysis
AU Nielsen, Simon Feldbk; Nielsen, Elsebet Ostergaard; Olsen, Gunnar M.; Liljefors, Tommy; Peters, Dan
CS NeuroSearch A/S, Ballerup, DK-2750, Den.
SO Journal of Medicinal Chemistry (2000), 43(11), 2217-2226
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB In the past few years the focus on central acetylcholine receptors has shifted from compds. with affinity for muscarinic acetylcholine receptors (mAChR) to compds. with affinity for nicotinic acetylcholine receptors (nAChR). The therapeutic potential includes treatment of a variety of diseases, e.g., Alzheimer's disease, Parkinson's disease, and Tourette's syndrome. This work describes the synthesis of six novel series of potent ligands with nanomolar affinity for the .alpha.4.beta.2 nAChR subtype. Structure-activity relationship (SAR) was evaluated by the calcn. of a 3D-QSAR model. 3D-QSAR anal. of the compds. using the GRID/GOLPE methodol. resulted in a model of high quality (R2 = 0.97, Q2 = 0.81). The coeff. plots reveal that the steric interactions between the target and our compds. are of major importance for the affinity. Bulky substituents in the 6-position of the pyridine ring will reduce the affinity of the compds., whereas bulky ring systems including a sp3-nitrogen will increase the affinity of the compds.
IT **223796-20-1P 223796-21-2P 223796-26-7P**
223796-36-9P 223796-37-0P
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(synthesis, receptor binding, and 3D-QSAR anal. of novel potent ligands for the central nAChR)
RN 223796-20-1 CAPLUS
CN 1H-1,4-Diazepine, hexahydro-1-(3-pyridinyl)- (9CI) (CA INDEX NAME)



RN 223796-21-2 CAPLUS
CN 1H-1,4-Diazepine, hexahydro-1-(3-pyridinyl)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

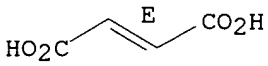
CRN 223796-20-1
CMF C10 H15 N3



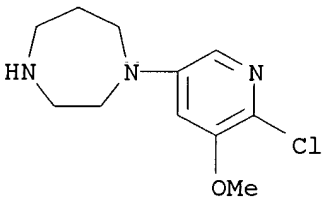
CM 2

CRN 110-17-8
CMF C4 H4 O4

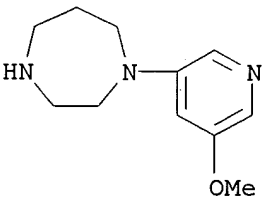
Double bond geometry as shown.



RN 223796-26-7 CAPLUS
CN 1H-1,4-Diazepine, 1-(6-chloro-5-methoxy-3-pyridinyl)hexahydro- (9CI) (CA INDEX NAME)



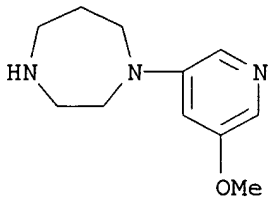
RN 223796-36-9 CAPLUS
CN 1H-1,4-Diazepine, hexahydro-1-(5-methoxy-3-pyridinyl)- (9CI) (CA INDEX NAME)



RN 223796-37-0 CAPLUS
CN 1H-1,4-Diazepine, hexahydro-1-(5-methoxy-3-pyridinyl)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

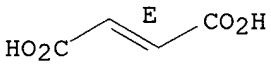
CRN 223796-36-9
CMF C11 H17 N3 O



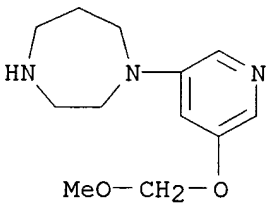
CM 2

CRN 110-17-8
CMF C4 H4 O4

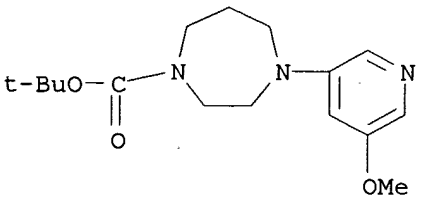
Double bond geometry as shown.



IT **223796-74-5P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(synthesis, receptor binding, and 3D-QSAR anal. of novel potent ligands for the central nAChR)
RN 223796-74-5 CAPLUS
CN 1H-1,4-Diazepine, hexahydro-1-[5-(methoxymethoxy)-3-pyridinyl]- (9CI) (CA INDEX NAME)



IT **223797-63-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis, receptor binding, and 3D-QSAR anal. of novel potent ligands for the central nAChR)
RN 223797-63-5 CAPLUS
CN 1H-1,4-Diazepine-1-carboxylic acid, hexahydro-4-(5-methoxy-3-pyridinyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2003 ACS
AN 1999:299480 CAPLUS
DN 130:325154
TI Preparation of N-pyridylpiperazines and analogs as nicotinic receptor ligands
IN Peters, Dan; Olsen, Gunnar M.; Nielsen, Simon Feldbaek; Nielsen, Elsebet Ostergaard
PA Neurosearch A/S, Den.
SO PCT Int. Appl., 68 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9921834	A1	19990506	WO 1998-DK465	19981027
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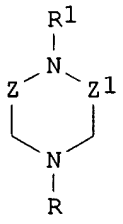
	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	CA 2306093	AA	19990506	CA 1998-2306093	19981027
	AU 9897368	A1	19990517	AU 1998-97368	19981027
	AU 744539	B2	20020228		
	ZA 9809771	A	19990929	ZA 1998-9771	19981027
	EP 1027336	A1	20000816	EP 1998-951286	19981027
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	BR 9813279	A	20000822	BR 1998-13279	19981027
	EE 200000178	A	20010416	EE 2000-20000017819981027	
	JP 2001521025	T2	20011106	JP 2000-517946	19981027
	NZ 503520	A	20020828	NZ 1998-503520	19981027
	NO 2000002132	A	20000426	NO 2000-2132	20000426
PRAI	DK 1997-1225	A	19971027		
	DK 1998-409	A	19980324		
	DK 1998-796	A	19980619		
	WO 1998-DK465	W	19981027		

OS MARPAT 130:325154
GI



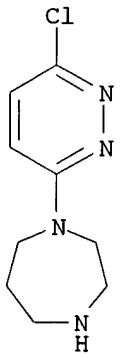
I

AB Title compds. [I; R = H, (cyclo)alkyl, aralkyl; R1 = C6H4R2 or

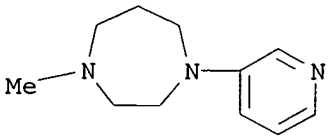
(un)substituted heteroaryl; R2 = NH2, NO2, OH, alkoxy; Z = (CH2)0-2; Z1 = (CH2)1-3] were prepd. Thus, 1-tert-butoxycarbonylpiperazine was N-arylated by 3-bromopyridine and the deprotected product N-methylated to give I (R = Me, R1 = 3-pyridyl, Z = Z1 = CH2). Data for biol activity of I were given.

IT **100224-61-1P 223795-46-8P 223796-15-4P**
223796-16-5P 223796-20-1P 223796-21-2P
223796-26-7P 223796-36-9P 223796-37-0P
223796-62-1P 223796-74-5P 223796-75-6P
223796-79-0P 223796-90-5P 223796-91-6P
223796-92-7P 223796-93-8P 223797-08-8P
223797-23-7P 223797-24-8P 223797-25-9P
223797-44-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-pyridylpiperazines and analogs as nicotinic receptor ligands)

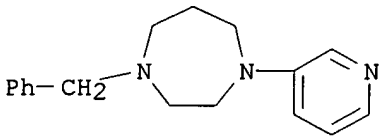
RN 100224-61-1 CAPLUS
CN 1H-1,4-Diazepine, 1-(6-chloro-3-pyridazinyl)hexahydro- (9CI) (CA INDEX NAME)



RN 223795-46-8 CAPLUS
CN 1H-1,4-Diazepine, hexahydro-1-methyl-4-(3-pyridinyl)- (9CI) (CA INDEX NAME)



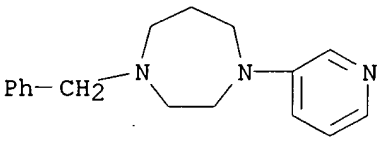
RN 223796-15-4 CAPLUS
CN 1H-1,4-Diazepine, hexahydro-1-(phenylmethyl)-4-(3-pyridinyl)- (9CI) (CA INDEX NAME)



RN 223796-16-5 CAPLUS
CN 1H-1,4-Diazepine, hexahydro-1-(phenylmethyl)-4-(3-pyridinyl)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

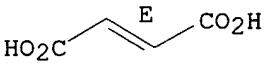
CRN 223796-15-4
CMF C17 H21 N3



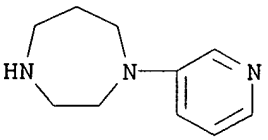
CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



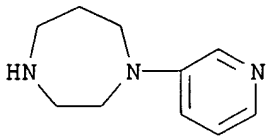
RN 223796-20-1 CAPLUS
CN 1H-1,4-Diazepine, hexahydro-1-(3-pyridinyl)- (9CI) (CA INDEX NAME)



RN 223796-21-2 CAPLUS
CN 1H-1,4-Diazepine, hexahydro-1-(3-pyridinyl)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

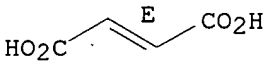
CRN 223796-20-1
CMF C10 H15 N3



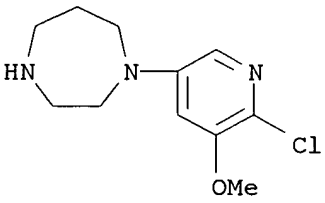
CM 2

CRN 110-17-8
CMF C4 H4 O4

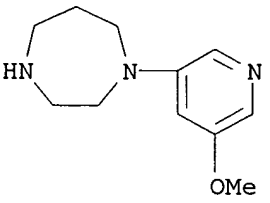
Double bond geometry as shown.



RN 223796-26-7 CAPLUS
CN 1H-1,4-Diazepine, 1-(6-chloro-5-methoxy-3-pyridinyl)hexahydro- (9CI) (CA INDEX NAME)



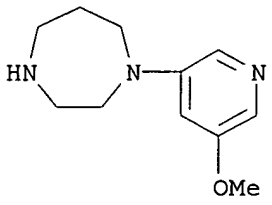
RN 223796-36-9 CAPLUS
CN 1H-1,4-Diazepine, hexahydro-1-(5-methoxy-3-pyridinyl)- (9CI) (CA INDEX NAME)



RN 223796-37-0 CAPLUS
CN 1H-1,4-Diazepine, hexahydro-1-(5-methoxy-3-pyridinyl)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

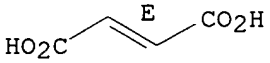
CRN 223796-36-9
CMF C11 H17 N3 O



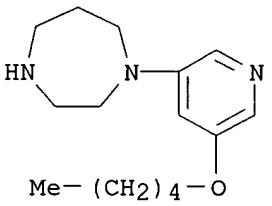
CM 2

CRN 110-17-8
CMF C4 H4 O4

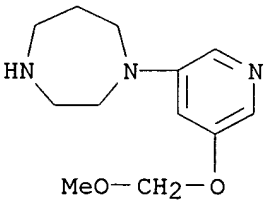
Double bond geometry as shown.



RN 223796-62-1 CAPLUS
CN 1H-1,4-Diazepine, hexahydro-1-[5-(pentyloxy)-3-pyridinyl]- (9CI) (CA INDEX NAME)



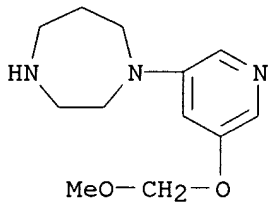
RN 223796-74-5 CAPLUS
CN 1H-1,4-Diazepine, hexahydro-1-[5-(methoxymethoxy)-3-pyridinyl]- (9CI) (CA INDEX NAME)



RN 223796-75-6 CAPLUS
CN 1H-1,4-Diazepine, hexahydro-1-[5-(methoxymethoxy)-3-pyridinyl]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

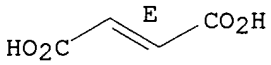
CRN 223796-74-5
CMF C12 H19 N3 O2



CM 2

CRN 110-17-8
CMF C4 H4 O4

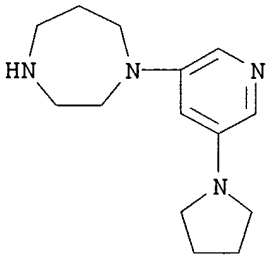
Double bond geometry as shown.



RN 223796-79-0 CAPLUS
CN 1H-1,4-Diazepine, hexahydro-1-[5-(1-pyrrolidinyl)-3-pyridinyl]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

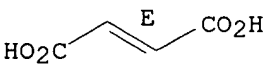
CRN 223796-78-9
CMF C14 H22 N4



CM 2

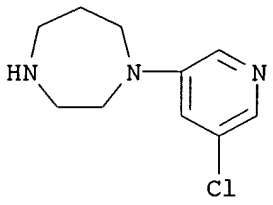
CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



RN 223796-90-5 CAPLUS
CN 1H-1,4-Diazepine, 1-(5-chloro-3-pyridinyl)hexahydro- (9CI) (CA INDEX

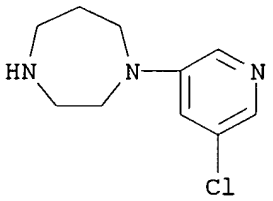
NAME)



RN 223796-91-6 CAPLUS
CN 1H-1,4-Diazepine, 1-(5-chloro-3-pyridinyl)hexahydro-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

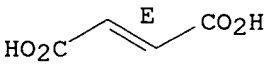
CRN 223796-90-5
CMF C10 H14 Cl N3



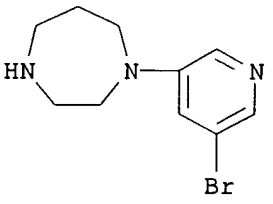
CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



RN 223796-92-7 CAPLUS
CN 1H-1,4-Diazepine, 1-(5-bromo-3-pyridinyl)hexahydro- (9CI) (CA INDEX NAME)

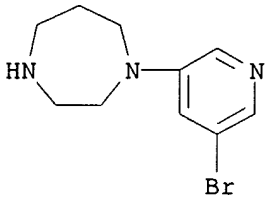


RN 223796-93-8 CAPLUS
CN 1H-1,4-Diazepine, 1-(5-bromo-3-pyridinyl)hexahydro-, (2E)-2-butenedioate

(1:1) (9CI) (CA INDEX NAME)

CM 1

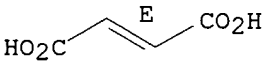
CRN 223796-92-7
CMF C10 H14 Br N3



CM 2

CRN 110-17-8
CMF C4 H4 O4

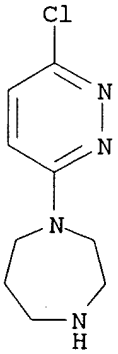
Double bond geometry as shown.



RN 223797-08-8 CAPLUS
CN 1H-1,4-Diazepine, 1-(6-chloro-3-pyridazinyl)hexahydro-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

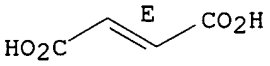
CRN 100224-61-1
CMF C9 H13 Cl N4



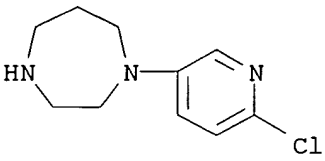
CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



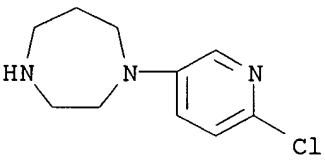
RN 223797-23-7 CAPLUS
CN 1H-1,4-Diazepine, 1-(6-chloro-3-pyridinyl)hexahydro- (9CI) (CA INDEX NAME)



RN 223797-24-8 CAPLUS
CN 1H-1,4-Diazepine, 1-(6-chloro-3-pyridinyl)hexahydro-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

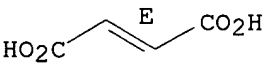
CRN 223797-23-7
CMF C10 H14 Cl N3



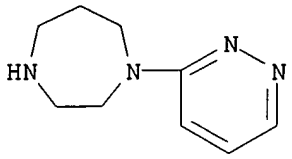
CM 2

CRN 110-17-8
CMF C4 H4 O4

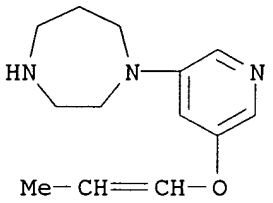
Double bond geometry as shown.



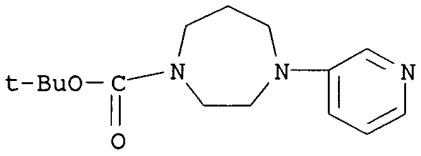
RN 223797-25-9 CAPLUS
CN 1H-1,4-Diazepine, hexahydro-1-(3-pyridazinyl)- (9CI) (CA INDEX NAME)



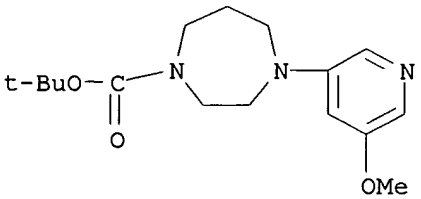
RN 223797-44-2 CAPLUS
CN 1H-1,4-Diazepine, hexahydro-1-[5-(1-propenyloxy)-3-pyridinyl]- (9CI) (CA INDEX NAME)



IT **223797-48-6P 223797-63-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of N-pyridylpiperazines and analogs as nicotinic receptor ligands)
RN 223797-48-6 CAPLUS
CN 1H-1,4-Diazepine-1-carboxylic acid, hexahydro-4-(3-pyridinyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 223797-63-5 CAPLUS
CN 1H-1,4-Diazepine-1-carboxylic acid, hexahydro-4-(5-methoxy-3-pyridinyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2003 ACS
AN 1986:129918 CAPLUS
DN 104:129918
TI Anti-virally active pyridazinamines
IN Stokbroekx, Raymond Antoine; Van der Aa, Marcel Jozef Maria; Willems, Joannes Josephus Maria; Luyckx, Marcel Gerebernus Maria
PA Janssen Pharmaceutica N.V., Belg.
SO Eur. Pat. Appl., 76 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 156433	A2	19851002	EP 1985-200384	19850315
	EP 156433	A3	19860723		
	EP 156433	B1	19910227		
	R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
	US 5001125	A	19910319	US 1985-702772	19850215
	AT 61050	E	19910315	AT 1985-200384	19850315
	CZ 277730	B6	19930317	CZ 1985-1952	19850320
	NO 8501167	A	19850927	NO 1985-1167	19850322
	NO 161257	B	19890417		
	NO 161257	C	19890726		
	ES 541521	A1	19860416	ES 1985-541521	19850322
	SU 1384198	A3	19880323	SU 1985-3867689	19850322
	DK 8501341	A	19850927	DK 1985-1341	19850325
	DK 166277	B	19930329		
	DK 166277	C	19930830		
	FI 8501177	A	19850927	FI 1985-1177	19850325
	FI 85373	B	19911231		
	FI 85373	C	19920410		
	AU 8540348	A1	19851003	AU 1985-40348	19850325
	AU 576563	B2	19880901		
	JP 60226862	A2	19851112	JP 1985-58636	19850325
	HU 37614	A2	19860123	HU 1985-1127	19850325
	HU 198010	B	19890728		
	ZA 8502235	A	19861126	ZA 1985-2235	19850325
	IL 74707	A1	19880531	IL 1985-74707	19850325
	CA 1238321	A1	19880621	CA 1985-477330	19850325
	PL 147465	B1	19890630	PL 1985-252562	19850325
	RO 91197	B3	19870630	RO 1985-118137	19850326
	US 5157035	A	19921020	US 1991-637091	19910103
	US 5292738	A	19940308	US 1992-929622	19920813
PRAI	US 1984-593444		19840326		
	US 1985-702772		19850215		
	EP 1985-200384		19850315		
	US 1991-637091		19910103		

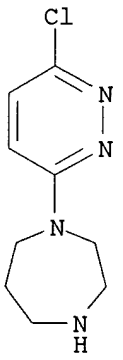
GI For diagram(s), see printed CA Issue.
AB The title compds. I [R1 = H, halo, 1H-imidazol-1-yl, alkyloxy, aryloxy, aralkoxy, alkylthio, arylthio, HO, HS, amino, alkylsulfinyl, alkylsulfonyl, cyano, alkoxycarbonyl, alkanoyl, alkyl; R2, R3 = H, alkyl; R2R3 = CH:CHCH:CH; X = CH:NCH:CH2, optionally alkyl- or aryl-substituted CmH2mNR4CnH2n,CmH2mCR5R6CnH2n, Cm-1H2(m-1)CR7:CR8CnH2n; R4 = H, alkyl, aryl, thiazolyl, pyrimidinyl, quinolinyl, etc.; R5 = H, alkyl, aryl, HO, alkyloxy, etc.; R6 = H, alkyl, aryl, indolyl, pyridinyl, etc.; R7, R8 = H, alkyl, aryl, aralkyl, pyridinyl; aryl = (un)substituted Ph; m,n = 1-4; m+n = 3-5] were prepd. Thus, 3,6-dichloropyridazine was treated with

1,2,3,6-tetrahydro-4-(3-methylphenyl)pyridine to give pyridinylpyridazine II, which in the Rhinovirus Cytopathic Effect Test gave 0.006 .mu.g/mL as the lowest concn. necessary to inhibit .gtoreq.75% of the cytopathic effect of human rhinovirus. Oral drops were prepd. by dissolving 500 g I in 0.5 L MeCHOHCO2H and 1.5 L polypropylene glycol at 60-80.degree., cooling to 30-40.degree., adding 35 L polyethylene glycol, mixing well, adding 1750 g Na saccharin in 2.5 L purified H2O and 2.5 L cocoa flavor, and finally polyethylene glycol to 50 L to provide a soln. comprising 10 mg I/mL.

IT **100224-61-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as virucide)

RN 100224-61-1 CAPLUS

CN 1H-1,4-Diazepine, 1-(6-chloro-3-pyridazinyl)hexahydro- (9CI) (CA INDEX NAME)



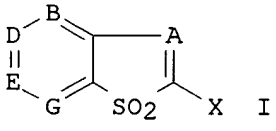
=> d bib abs hitstr 1-2

L68 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS
AN 2003:42270 CAPLUS
DN 138:89958
TI Preparation of benzothiophene and benzothiazole compounds as cholinergic and monoamine receptor modulators
IN Peters, Dan; Olsen, Gunnar M.; **Nielsen, Elsebet Ostergaard;** Ahring, Philip K.; Jorgensen, Tino Dyhring
PA Neurosearch A/S, Den.
SO PCT Int. Appl., 44 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

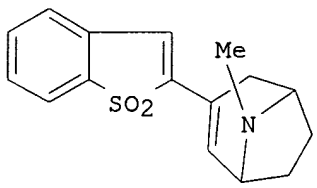
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003004493	A1	20030116	WO 2002-DK460	20020702

PI
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI DK 2001-1064 A 20010706
OS MARPAT 138:89958
GI



I



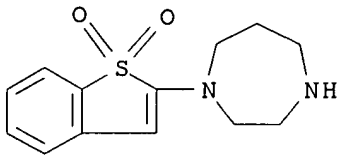
II

AB Novel compds. of formula I [A, B, D, E, G = C, N; X = heterocycle] are prepd. that are found to be cholinergic ligands at the nicotinic acetylcholine receptors and modulators of the monoamine receptors and transporters. Due to their pharmacol. profile the compds. of the invention may be useful for the treatment of diseases or disorders as diverse as those related to the cholinergic system of the central nervous system (CNS), the peripheral nervous system (PNS), diseases or disorders related to smooth muscle contraction, endocrine diseases or disorders, diseases or disorders related to neuro-degeneration, diseases or disorders related to inflammation, pain, and withdrawal symptoms caused by the termination of abuse of chem. substances. Thus, was prepd. and inhibited 3H-.alpha.-bungarotoxine binding in rat brain with IC50 of 0.018 .mu.M.

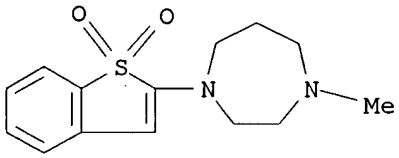
IT **484650-82-0P 484650-83-1P 484650-84-2P**
484650-85-3P 484651-02-7P 484651-03-8P
484651-04-9P 484651-05-0P
RL: DGN (Diagnostic use); PAC (Pharmacological activity); SPN (Synthetic

preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of benzothiophene and benzothiazole compds. as cholinergic and monoamine receptor modulators)

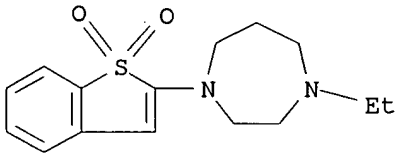
RN 484650-82-0 CAPLUS
CN 1H-1,4-Diazepine, 1-(1,1-dioxidobenzo[b]thien-2-yl)hexahydro- (9CI) (CA INDEX NAME)



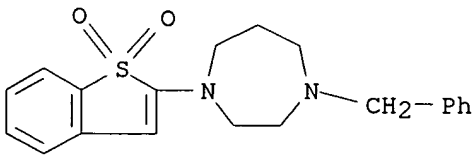
RN 484650-83-1 CAPLUS
CN 1H-1,4-Diazepine, 1-(1,1-dioxidobenzo[b]thien-2-yl)hexahydro-4-methyl- (9CI) (CA INDEX NAME)



RN 484650-84-2 CAPLUS
CN 1H-1,4-Diazepine, 1-(1,1-dioxidobenzo[b]thien-2-yl)-4-ethylhexahydro- (9CI) (CA INDEX NAME)

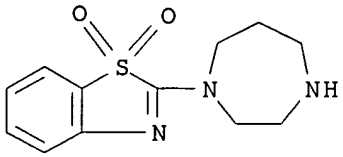


RN 484650-85-3 CAPLUS
CN 1H-1,4-Diazepine, 1-(1,1-dioxidobenzo[b]thien-2-yl)hexahydro-4-(phenylmethyl)- (9CI) (CA INDEX NAME)

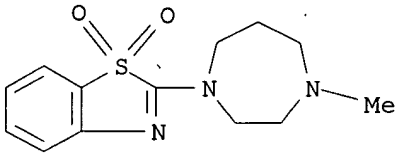


RN 484651-02-7 CAPLUS
CN Benzothiazole, 2-(hexahydro-1H-1,4-diazepin-1-yl)-, 1,1-dioxide (9CI) (CA

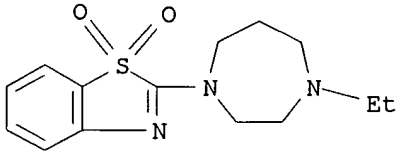
INDEX NAME)



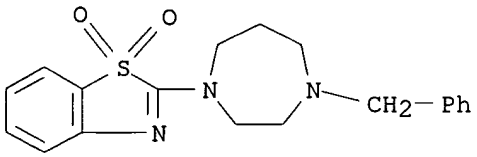
RN 484651-03-8 CAPLUS
CN Benzothiazole, 2-(hexahydro-4-methyl-1H-1,4-diazepin-1-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)



RN 484651-04-9 CAPLUS
CN Benzothiazole, 2-(4-ethylhexahydro-1H-1,4-diazepin-1-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)



RN 484651-05-0 CAPLUS
CN Benzothiazole, 2-[hexahydro-4-(phenylmethyl)-1H-1,4-diazepin-1-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

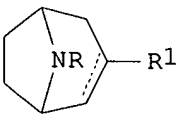


RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L68 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS
AN 2000:384193 CAPLUS
DN 133:30663
TI Preparation of 8-azabicyclo[3.2.1]oct-2-ene and -octane derivatives as cholinergic ligands at the nicotinic Acetyl Choline Receptors (nAChR)
IN Peters, Dan; Olsen, Gunnar M.; Nielsen, Simon Feldbaek; **Nielsen, Elsebet Ostergaard**
PA Neurosearch A/S, Den.
SO PCT Int. Appl., 58 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000032600	A1	20000608	WO 1999-DK661	19991126
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	CA 2342621	AA	20000608	CA 1999-2342621	19991126
	EP 1133494	A1	20010919	EP 1999-973031	19991126
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	JP 2002531456	T2	20020924	JP 2000-585242	19991126
	US 2002035122	A1	20020321	US 2001-864367	20010525
PRAI	DK 1998-1570	A	19981127		
	WO 1999-DK661	W	19991126		

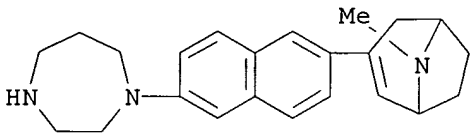
OS MARPAT 133:30663
GI



I

AB The title compds. [I; R = H, alkyl, alkenyl, etc.; R1 = COR2, (un)substituted mono- or polycyclic aryl, (un)substituted (un)satd. 5-6 membered heterocyclyl, etc.; R2 = H, alkyl, alkenyl, etc.] and their salts which are found to be cholinergic ligands at the nicotinic Acetyl Choline Receptors (no data) and may be useful for the treatment of diseases or disorders as diverse as those related to the cholinergic system of the central nervous system (CNS), diseases or disorders related to smooth muscle contraction, endocrine diseases or disorders, diseases or disorders related to neurodegeneration, diseases or disorders related to inflammation, pain, and withdrawal symptoms caused by the termination of abuse of chem. substances, were prepd. E.g., a 2-step synthesis of (.+-.)-8-azabicyclo[3.2.1]oct-2-ene I.fumarate [R = Me; R1 = 6-methoxy-2-naphthyl] was given. Compds. I may also be useful as radioligands for in vivo receptor imaging (neuroimaging).

IT **273403-29-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 8-azabicyclo[3.2.1]oct-2-ene and -octane derivs. as cholinergic ligands at the nicotinic Acetyl Choline Receptors (nAChR))
RN 273403-29-5 CAPLUS
CN 8-Azabicyclo[3.2.1]oct-2-ene, 3-[6-(hexahydro-1H-1,4-diazepin-1-yl)-2-naphthalenyl]-8-methyl- (9CI) (CA INDEX NAME)



RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT